

APPROVED	O G. FIG.:
BY	CLASS
DRAFTSMAN	SUBCLASS

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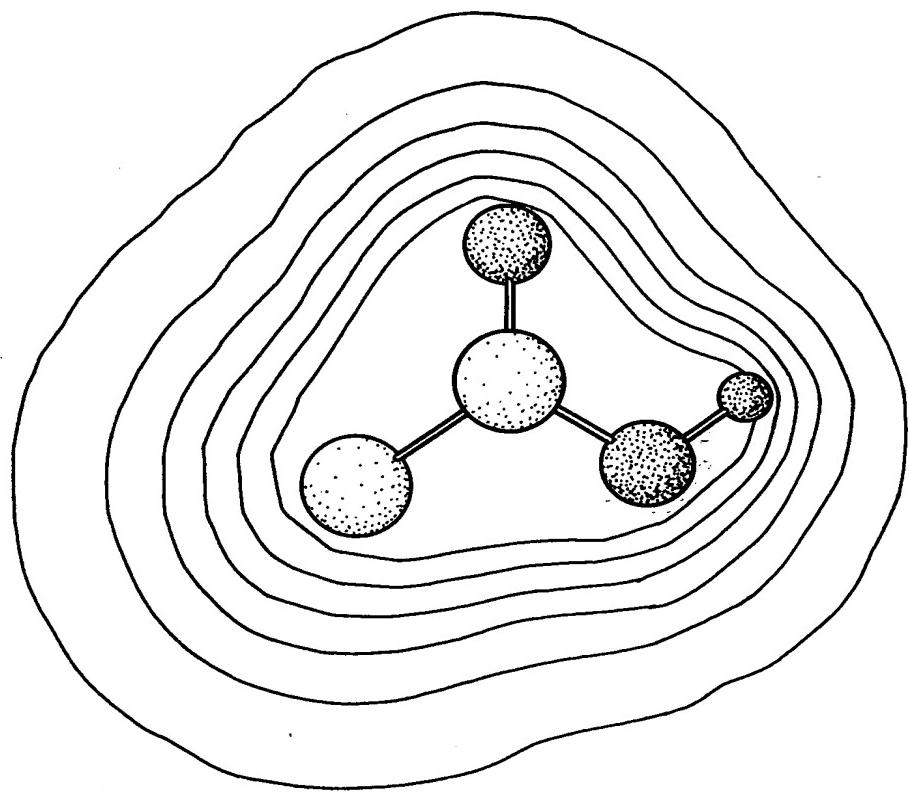


FIG.1

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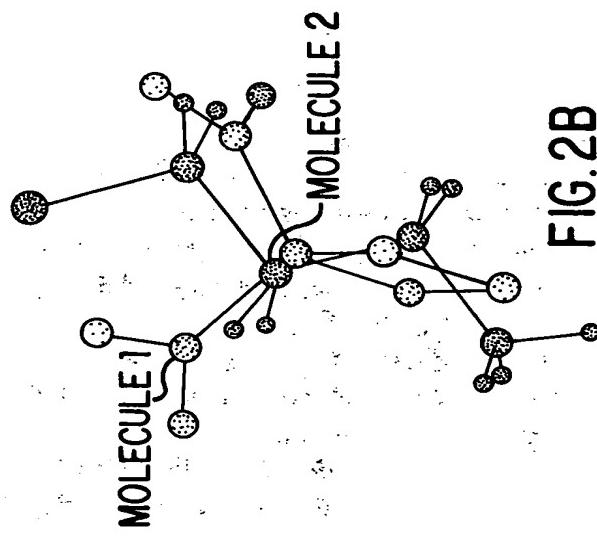


FIG. 2B

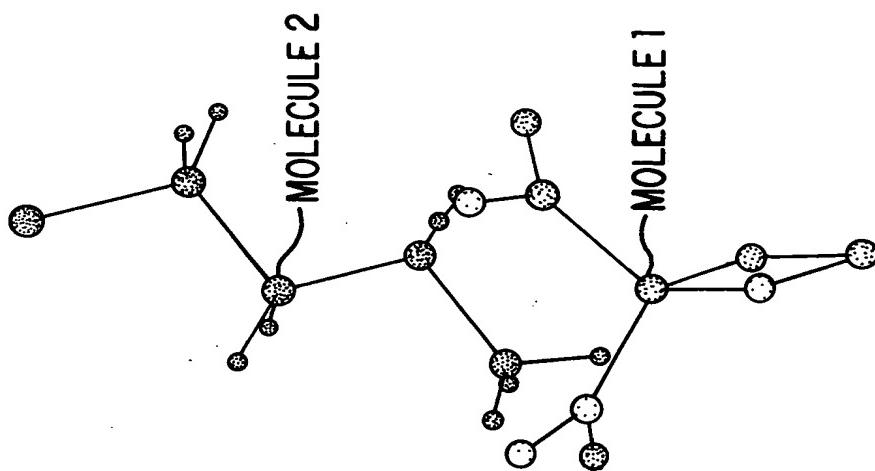


FIG. 2A

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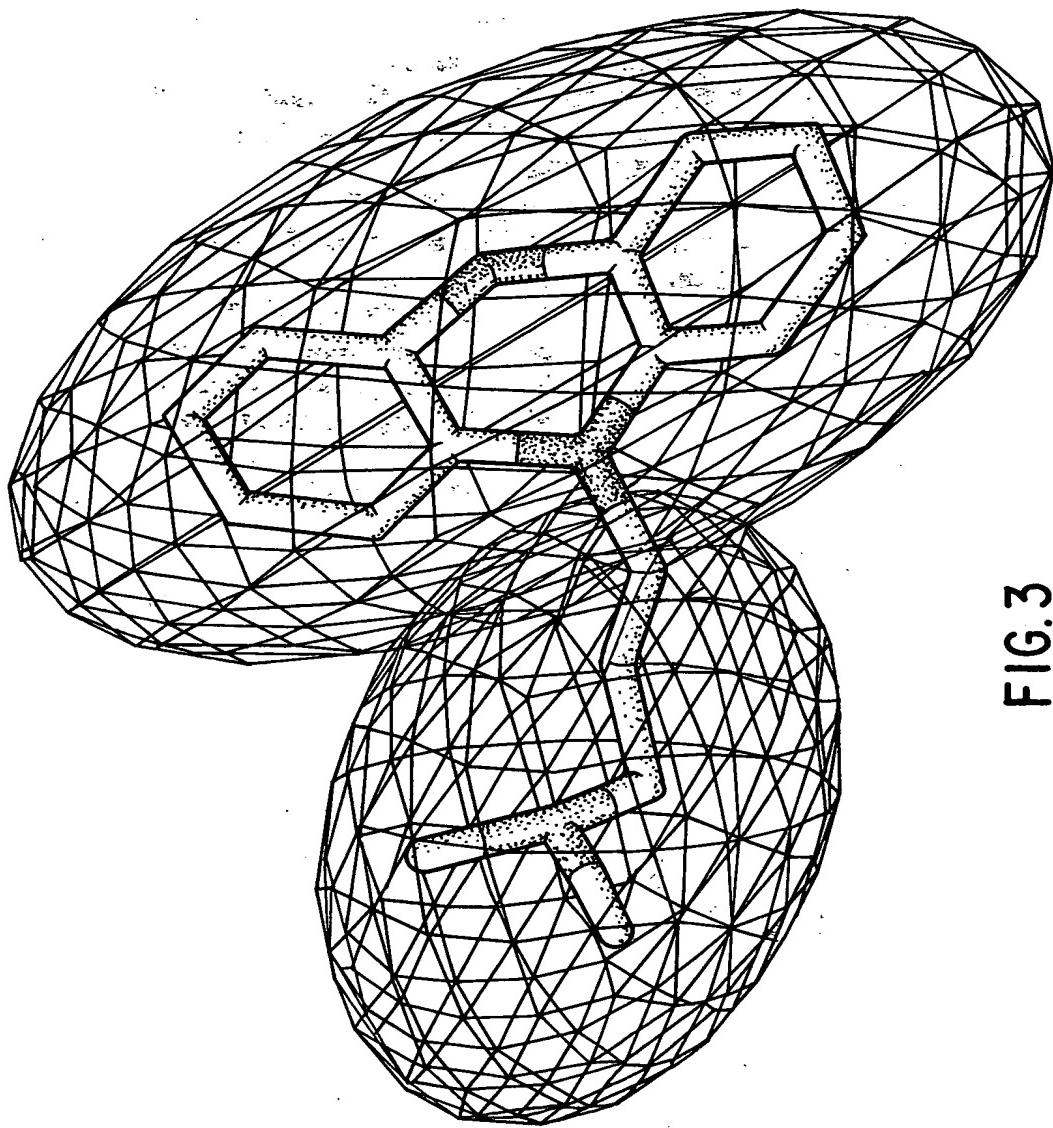


FIG. 3

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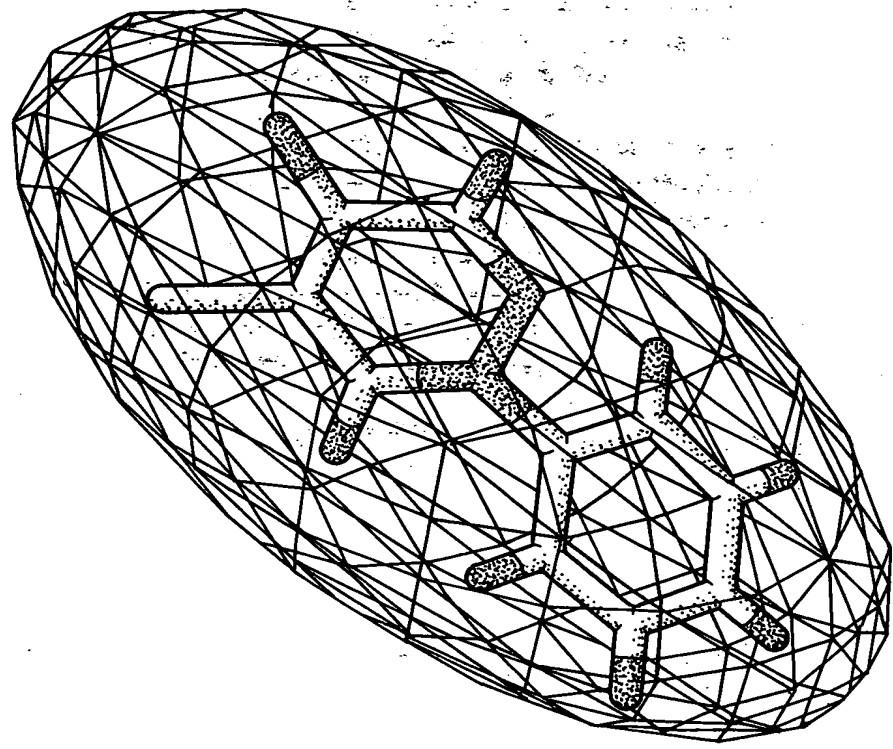


FIG.4A

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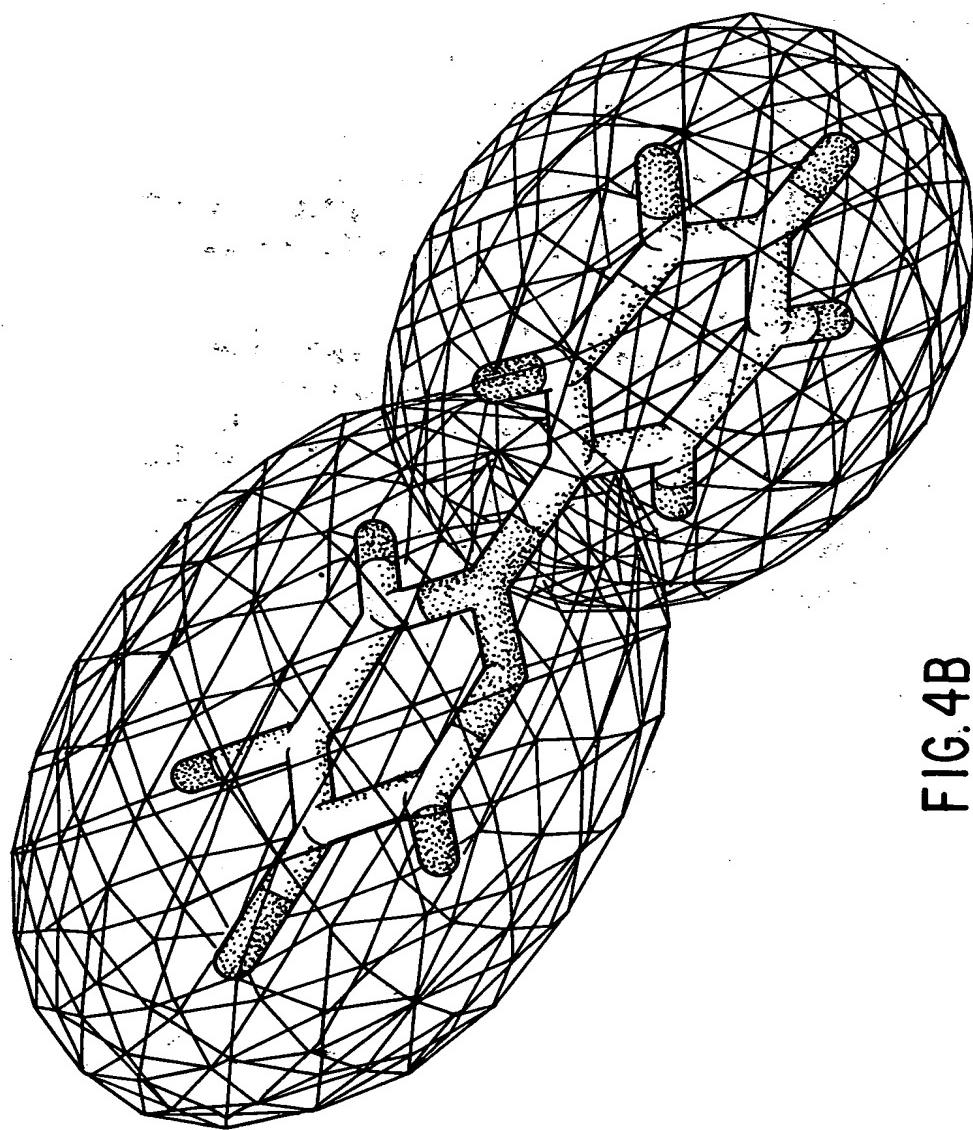


FIG. 4B

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BY	CLASS	SUBCLASS
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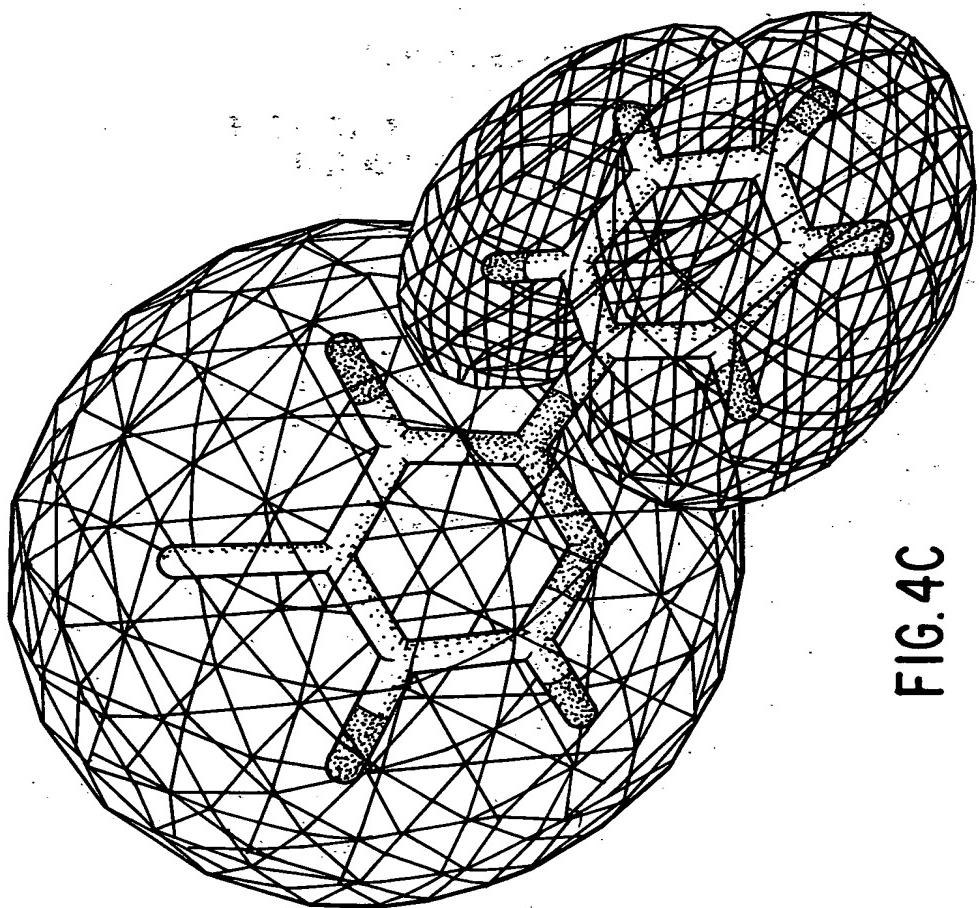


FIG. 4C

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APPROVED BY	O. G. FIG.
	CLASS
DRAFTSMAN	SUBCLASS

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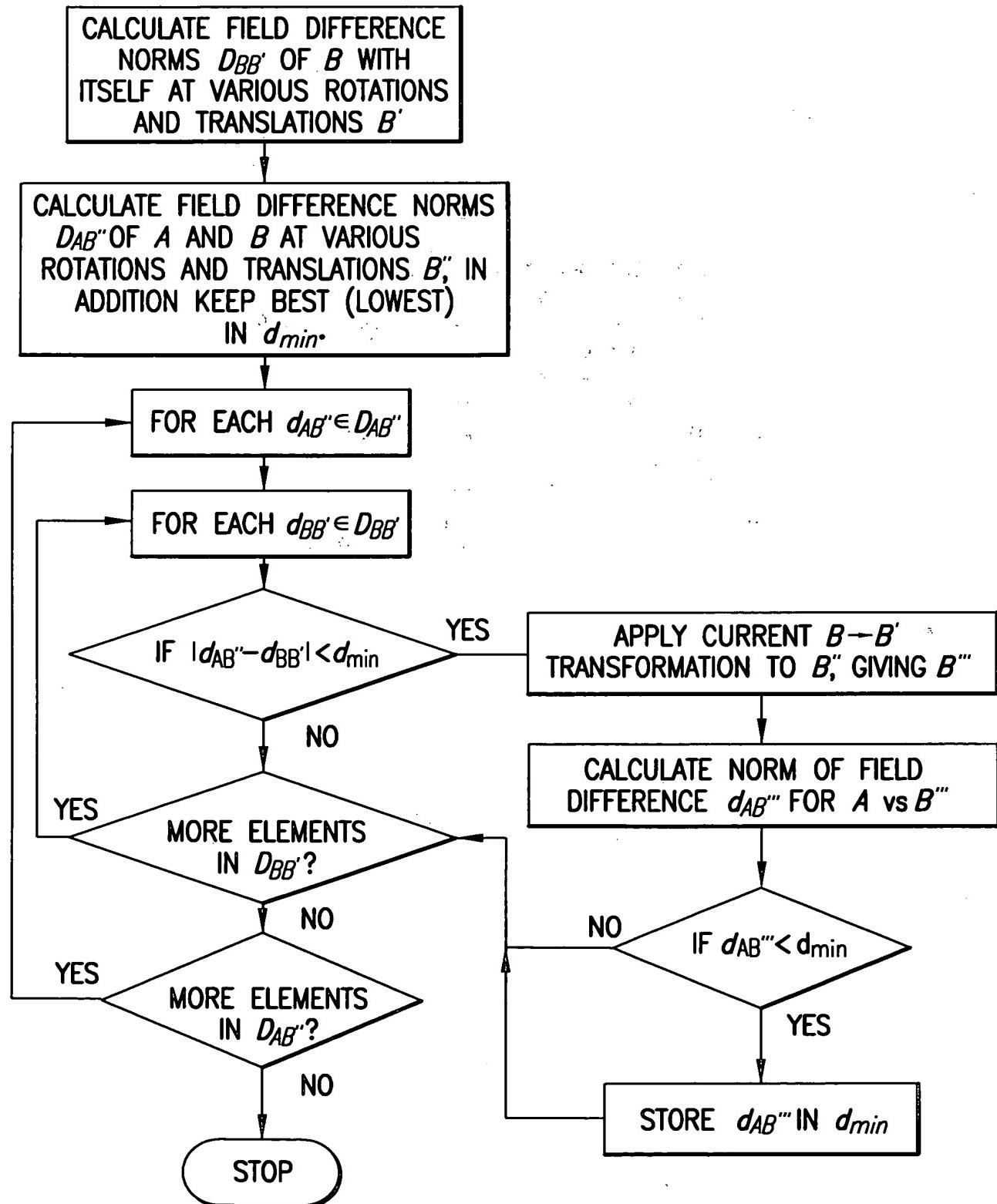


FIG.5

APPROVED BY DRAFTSMAN	O G. FIG. CLASS	SUBCLASS
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CHOOSE A STARTING SET OF $N \geq 2$ STRUCTURES FROM A LARGER COLLECTION. CHOOSE A FIELD PROPERTY, i.e. STERIC, ELECTROSTATIC.

FOR EACH PAIR OF STRUCTURES, FIND THE MINIMAL VALUE OF THE NORM OF THEIR FIELD DIFFERENCE, AND STORE IN THE DISTANCE MATRIX D.

CONSTRUCT METRIC MATRIX G FROM D

DIAGONALIZE G, FIND EIGENVALUES

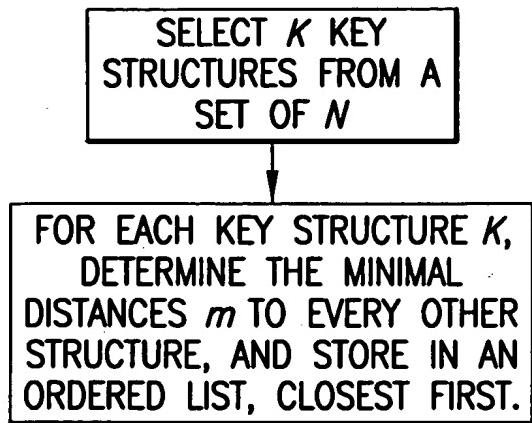
FIND COORDINATES OF STRUCTURES IN N -DIMENSIONAL SHAPE SPACE.

DISCARD UNIMPORTANT COORDINATES (AXES) TO REDUCE DIMENSIONALITY FROM N TO M SUCH THAT DISTANCES IN D ARE STILL REPRODUCED TO WITHIN TOLERANCE τ .

M -DIMENSIONAL SHAPE SPACE,
 $M \leq N$, DISTANCE TOLERANCE τ ,
FOR CHOSEN FIELD PROPERTY.

FIG.6

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FIND WHICH KEY STRUCTURE K HAS THE SMALLEST MINIMAL DISTANCE X TO A TEST STRUCTURE. STORE X IN $BEST$.

STARTING AT THE TOP OF K 'S LIST OF DISTANCES m ...

YES

$m > X + BEST?$

NO

FIND MINIMAL DISTANCE d FROM THE TEST STRUCTURE TO STRUCTURE CORRESPONDING TO CURRENT m .

NO

$d < BEST?$

YES

STORE d IN $BEST$.

STOP

NO

MORE ITEMS IN LIST?

YES

GET NEXT m .

FIG.7B